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WKB corrections to the energy splitting in double–well potentials

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Abstract. By using the WKB quantization we deduce an analytical formula for the energy splitting in a double–well potential which is the usual Landau formula with additional quantum corrections. Then we analyze the accuracy of our formula for the double square well potential and the parabolic double–well potential.

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In this paper we analyze the energy splitting in a generic one–dimensional double–well potential. By using the WKB quantization we deduce an analytical formula for the energy splitting which is the usual Landau (1973) formula with additional quantum corrections. The formula is based on a linear approximation of the potential near the turning points. We study the validity of this formula for the double square well potential and then we discuss the case of a parabolic double–well potential.

Let us consider a one–dimensional system with Hamiltonian

$$H = \frac{p^2}{2m} + V(x) \ , \tag{1}$$

where $V(-x) = V(x)$ is a symmetric double–well potential. The stationary Schrödinger equation of the system reads

$$\hat{H}\psi(x) = (-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(x))\psi(x) = E\psi(x). \tag{2}$$

The Sturm–Liouville theorem (see, for example, Flügge, 1971) ensures that for one–dimensional systems there are no degeneracies in the spectrum. Let ψ_1 and ψ_2 be two eigenfunctions of the Schrödinger equation

$$\hat{H}\psi_1 = E_1\psi_1 \quad \text{and} \quad \hat{H}\psi_2 = E_2\psi_2 \ , \tag{3}$$

such that $\psi_1(-x) = \psi_1(x)$ and $\psi_2(-x) = -\psi_2(x)$ and $E_1 \simeq E_2$. To calculate the splitting $\Delta E = E_2 - E_1$, we multiply the first equation by ψ_2 and the second by ψ_1 and then we subtract the two resulting equations. By integrating from 0 to ∞ we find

$$\Delta E = \frac{\hbar^2}{2m}\frac{\psi_1(0)\psi'_2(0) - \psi'_1(0)\psi_2(0)}{\int_0^\infty \psi_1(x)\psi_2(x)dx} \ . \tag{4}$$

We write the eigenfunctions ψ_1 and ψ_2 in terms of the right–localized function

$$\psi_0(x) = \frac{1}{\sqrt{2}}(\psi_1(x) + \psi_2(x)) \ . \tag{5}$$

It is easy to show that $E_0 =< \psi_0|\hat{H}|\psi_0 >= \frac{1}{2}(E_1 + E_2)$. Then, with the approximation

$$\int_0^\infty \psi_1(x)\psi_2(x)dx \simeq \frac{1}{2}\int_0^\infty \psi_0^2(x)dx = \frac{1}{2} \ , \tag{6}$$

we get

$$\Delta E = \frac{2\hbar^2}{m}\psi_0(0)\psi'_0(0) \ , \tag{7}$$

which is the starting formula to calculate the energy splitting. One should observe that this quantity is always positive, because the tail of the right localized eigenfunction $\psi_0(x)$ at $x = 0$ has the same sign for $\psi_0(0)$ and its derivative $\psi'_0(0)$. Another way to see this is to realize that because of Sturm-Liouville theorem there are no degeneracies and that implies that all pairs of almost degenerate states, from the ground state up, are grouped by odd state above the even state.

To determine the function ψ_0 we perform a WKB expansion of the Schrödinger equation. We observe that a generic eigenfunction ψ of the Schrödinger equation can always be written as

$$\psi(x) = \exp\,(\frac{i}{\hbar}\sigma(x)) \ , \tag{8}$$

where the phase $\sigma(x)$ is a complex function that satisfies the differential equation

$$\sigma'^2(x) + (\frac{\hbar}{i})\sigma''(x) = 2m(E - V(x)) \ . \tag{9}$$

The WKB expansion for the phase is given by

$$\sigma(x) = \sum_{k=0}^{\infty} (\frac{\hbar}{i})^k \sigma_k(x) \ . \tag{10}$$

Substituting (10) into (9) and comparing like powers of $\hbar$ gives the recursion relation ($n > 0$) (see Bender, Olaussen and Wang, 1977)

$$\sigma'^2_0 = 2m(E - V(x)), \quad \sum_{k=0}^{n} \sigma'_k \sigma'_{n-k} + \sigma''_{n-1} = 0 \ . \tag{11}$$

With the momentum $p = \sqrt{2m(E - V(x))}$ the first three orders in the WKB expansion give

$$\sigma'_0 = p \ , \quad \sigma'_1 = -\frac{p'}{2p} \ , \quad \sigma'_2 = \frac{p''}{4p^2} - \frac{3}{8}\frac{p'^2}{p^3} \ , \tag{12}$$

from which we obtain

$$\sigma_0 = \int p dx \ , \quad \sigma_1 = -\frac{1}{2} \ln p \ , \quad \sigma_2 = \frac{p'}{4p^2} + \frac{1}{8} \int \frac{p'^2}{p^3} dx \ . \tag{13}$$

It follows that, up to the second order, the wave–function can be written as

$$\psi(x) = \frac{1}{\sqrt{p}} \exp\Big(\frac{i}{\hbar} \int p dx - i\hbar [\frac{p'}{4p^2} + \frac{1}{8} \int \frac{p'^2}{p^3} dx]\Big) \ . \tag{14}$$

In particular, if we call a and b the two turning points corresponding to the energy E, the right localized wave–function ψ_0 is given by

$$\psi_0(0) = \frac{C}{\sqrt{|p|}} \exp\Big(-\frac{1}{\hbar} \int_x^a |p| dx + \hbar [\frac{1}{4} |\frac{p'}{p^2}| + \frac{1}{8} \int_x^a |\frac{p'^2}{p^3}| dx]\Big) \ , \tag{15}$$

for $0 < x < a$ (forbidden region), and

$$\psi_0(0) = \frac{C_1}{\sqrt{p}} \exp\Big(\frac{i}{\hbar} \int_a^x p dx - i\hbar [\frac{p'}{4p^2} + \frac{1}{8} \int_a^x \frac{p'^2}{p^3} dx]\Big) +$$

$$+ \frac{C_2}{\sqrt{p}} \exp\Big(- \frac{i}{\hbar} \int_a^x p dx + i\hbar [\frac{p'}{4p^2} + \frac{1}{8} \int_a^x \frac{p'^2}{p^3} dx] \Big) \ , \tag{16}$$

for $a < x < b$ (allowed region).

It is possible to write C_1 and C_2 in terms of C by imposing the uniqueness of the wave–function ψ_0 at the turning points. Following Landau (1973) we suppose that near the turning point $x = a$ it is possible to approximate the potential locally linearly by writing

$$E - V(x) = F_0(x - a) \ , \tag{17}$$

with $F_0 > 0$. In this case the connections at the turning point imply that

$$C_1 = C e^{i\frac{\pi}{4}} \quad \text{and} \quad C_2 = C e^{-i\frac{\pi}{4}} \ , \tag{18}$$

and the right localized function $\psi_0(x)$ can be written for $a < x < b$ as

$$\psi_0(x) = \frac{2C}{\sqrt{p}} \cos\Big(\frac{1}{\hbar} \int_a^x p dx - \hbar [\frac{p'}{4p^2} + \frac{1}{8} \int_a^x \frac{p'^2}{p^3} dx] + \frac{\pi}{4} \Big) \ . \tag{19}$$

To determine C we impose the normalization condition

$$1 = \int_0^\infty |\psi_0(x)|^2 dx \ , \tag{20}$$

from which we get

$$C = \frac{1}{2} [\int_a^b \frac{dx}{p}]^{-1/2} \ . \tag{21}$$

Here we have replaced the oscillatory $\cos^2(.)$ factor in the integrand by its average value $1/2$, because of the rapid oscillations at small value of $\hbar$. The final formula is given by

$$\Delta E = \Delta E_{Landau} \cdot \Delta E_{WKB} \ , \tag{22}$$

where

$$\Delta E_{Landau} = \frac{2\hbar C^2}{m} \exp\Big(- \frac{1}{\hbar} \int_{-a}^{a} |p| dx \Big) \tag{23}$$

is the usual Landau (1973) formula for the energy splitting and

$$\Delta E_{WKB} = (1 + \frac{\hbar^2}{4} |\frac{p''(0)}{p(0)^3}|) \exp\Big(\frac{\hbar}{8} \int_{-a}^{a} |\frac{p'^2}{p^3}| dx \Big) \tag{24}$$

is the first quantum correction. We note that higher–order WKB corrections quickly increase in complexity (Robnik and Salasnich, 1997) but, in principle, they can be calculated from the equation (11). It is important to stress that our formula is good if the potential is sufficiently smooth so that the linear approximation is valid near the turning points.

As an example, we consider the double square well potential. In this case the linear approximation of the potential near the turning point is not valid. The potential is given by

$$\begin{aligned} V(x) &= V_0 \qquad \text{for } |x| < a \\ V(x) &= 0 \qquad \text{for } a < x < b \\ V(x) &= \infty \qquad \text{for } |x| > b \end{aligned} \tag{25}$$

For this potential we have $p'(x) = p''(x) = 0$ for $-a < x < a$ and the corrections to the Landau (1973) formula are zero. A naive application of the splitting formula gives

$$\Delta E = \frac{2\hbar\sqrt{E}}{\sqrt{2m}(b-a)} \exp\Big(- \frac{2a}{\hbar} \sqrt{2m(V_0 - E)} \Big) \, . \tag{26}$$

This formula is not correct. In fact, by using the exact wave–function

$$\psi_0(0) = D \exp\Big(- \frac{1}{\hbar} \sqrt{2m(V_0 - E)} \Big) \, , \tag{27}$$

for $0 < x < a$ (forbidden region), and

$$\psi_0(0) = A \exp\Big(\frac{i}{\hbar}\sqrt{2m(E-V_0)}\Big) + B \exp\Big(-\frac{i}{\hbar}\sqrt{2m(E-V_0)}\Big)\,, \qquad (28)$$

for $a < x < b$ (allowed region), and by imposing the exact matching and normalization conditions (Flügge, 1971) we find

$$A = \frac{D}{2}(1 - i\sqrt{\frac{V_0-E}{E}}) \exp\big(\frac{a}{\hbar}\sqrt{2m(V_0-E)} - \frac{a}{\hbar}\sqrt{E}\Big)\,, \qquad (29)$$

$$B = \frac{D}{2}(1 + i\sqrt{\frac{V_0-E}{E}}) \exp\big(\frac{a}{\hbar}\sqrt{2m(V_0-E)} + \frac{a}{\hbar}\sqrt{E}\Big)\,, \qquad (30)$$

and

$$D^2 = \frac{2E}{V_0(b-a)} \exp\Big(-\frac{2a}{\hbar}\sqrt{2m(V_0-E)}\Big)\,. \qquad (31)$$

Then, by applying the equation (7), we obtain:

$$\Delta E = \frac{4\hbar E\sqrt{2m(V_0-E)}}{mV_0(b-a)} \exp\Big(-\frac{2a}{\hbar}\sqrt{2m(V_0-E)}\Big)\,. \qquad (32)$$

This is the exact energy splitting for the double square well potential. It differs by a factor $4\sqrt{E(V_0-E)}/V_0$ from the WKB result based on the connection formulae (18) which are not justified in the present case.

To conclude we study a potential where our WKB splitting formula can be applied. We consider the parabolic double–well potential given by

$$\begin{aligned} V(x) &= V_0 - x^2 \qquad \text{for } |x| < \sqrt{V_0} \\ V(x) &= 0 \qquad\quad \text{for } \sqrt{V_0} < x < b \\ V(x) &= \infty \qquad\quad \text{for } |x| > b \end{aligned} \qquad (33)$$

The turning points are at $x = \pm a$, where $a = \sqrt{V_0 - E}$. We observe that

$$\int_a^b \frac{dx}{p} = \int_{\sqrt{V_0-E}}^{\sqrt{V_0}} \frac{1}{\sqrt{2m(E-V_0+x^2)}} dx + \int_{\sqrt{V_0}}^{b} \frac{1}{\sqrt{2mE}} dx\,, \qquad (34)$$

and

$$|\frac{p''(0)}{p(0)^3}| = \frac{1}{2m(V_0 - E)^2} \ . \tag{35}$$

It follows that the energy splitting up to the second order in the WKB corrections of $\hbar$ reads

$$\Delta E = \frac{2\hbar C^2}{m}(1 + \frac{\hbar^2}{8m(V_0 - E)^2}) \exp\Big(- \frac{m\pi}{\hbar}(V_0 - E)\Big) \ , \tag{36}$$

where

$$C^2 = \frac{\sqrt{2m}}{2}\Big[\ln\Big(\frac{\sqrt{E} + \sqrt{V_0}}{\sqrt{V_0 - E}}\Big) + \frac{(b - \sqrt{V_0})}{\sqrt{E}}\Big]^{-1} \ . \tag{37}$$

In this work we have taken the first step towards a systematic improvement of the Landau formula (Landau and Lifshitz 1973), which is the semiclassical leading order energy level splitting formula for pairs of almost degenerate levels in double well potentials. We have calculated explicitly the quantum corrections up to the second order, given in equations (21-24). Our approach is based on the usual WKB expansion in 1-dim potentials, embodied in formulae (8-11). Thus the calculation of higher corrections can in principle be continued by the same method, although the structure of higher terms increases in complexity very quickly. We have also shown what happens in cases where the assumption implicit in the Landau formula (namely the linearity of the potential around the turning points) is not satisfied: We get a different result even in the leading semiclassical order, and this has been shown for the double square well potential in equations (26) and (32).

It is our goal to work out a more direct WKB approach to the solution of the same problem, by the contour integration technique, based on requiring

the single valuedness of the eigenfunction, as has been done in the case of a single well potential in (Robnik and Salasnich 1997). This is our future project.

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